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SEARCH REQUEST FORM

Scientific and Technical Information Center

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Requester's Full Name:	5. kuma	Exa	miner#:	Date:	1810a
Art Unit: \63\	Phone Number 308	2-45)9	Serial Number: 👄	9/635.21	6 10/230 135
Mail Box and Bldg/Room	Location: $\frac{90}{7A}$	07 Results Fo	ormat Preferred (circ	le):(PAPER) D	ISK E-MAIL
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If more than one search	is submitted, pleas	e prioritize sea	ırches in order of	need. ///	*****
Please provide a detailed stater					oe searched.
Include the elected species or s	structures, keywords, sync	onyms, acronyms, a	nd registry numbers, a	nd combine with th	he concept or
utility of the invention. Define				evant citations, aut	hors, etc, if
known. Please attach a copy of					
Title of Invention: 1	agonists of the	Mognesium	binding det	ect as them	apentic Ogents.
Inventors (please provide ful	Inames): Thert	· Clifton	WELLS	,	
Thirefitors (picase provide to			-		
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Earliest Priority Filing Da	•				
For Sequence Searches Only	Please include all pertinent	information (parent,	child, divisional, or issu	ed patent numbers)	along with the
appropriate serial number.					
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Species 1	Claim (15)				
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=> fil reg FILE 'REGISTRY' ENTERED AT 11:34:46 ON 12 FEB 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

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10 FEB 2002 STRUCTURE FILE UPDATES: HIGHEST RN 391197-12-9 DICTIONARY FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> d sta que 140 L11 STR

VAR G1=7-2 10-4/11-2 12-4/13-2 14-4/15-2 17-4/18-2 21-4 VAR G2=NH2/22/25 NODE ATTRIBUTES: CONNECT IS E1 RC AT CONNECT IS E1 RC AT CONNECT IS E1 RC AT

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 26

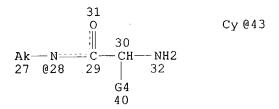
STEREO ATTRIBUTES: NONE

T.24 SCR 2016 OR 2026 OR 1997 OR 1841

L27 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 O

42

R 2043 OR 2054 4354 SEA FILE=REGISTRY SSS FUL L11 NOT (L24 OR L27) L29 L33 STR 37 6 0 0 NH-Ak Ak-N-Ak23 24 @25 26 @22 36 NH: - C - NH2 - CH2 C:--- G2 CH - Ak-2 3 . 4 034 35 38 G4



VAR G2=NH2/22/25
VAR G3=NH2/22/34/28
VAR G4=AK/43
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 43
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

84 SEA FILE=REGISTRY SUB=L29 CSS FUL L33 L35 12 SEA FILE=REGISTRY ABB=ON PLU=ON L35 AND (C6H14N2O OR L36 C5H10N2O) PLU=ON L36 AND PENTANAMIDE AND 1 SEA FILE=REGISTRY ABB=ON L37 AMINOMETHYL PLU=ON L36 AND PENTANAMIDE AND 5 L38 1 SEA FILE=REGISTRY ABB=ON AMINO 4 METHYL 1 SEA FILE=REGISTRY ABB=ON PLU=ON L36 AND BUTENAMIDE L39 3 SEA FILE=REGISTRY ABB=ON PLU=ON (L37 OR L38 OR L39) L40

=> d ide can tot 140

L40 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 214783-27-4 REGISTRY

CN Pentanamide, 3-(aminomethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C6 H14 N2 O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

$$\begin{array}{c|c} \text{O} & \text{CH}_2\text{--}\text{NH}_2 \\ \parallel & \parallel \\ \text{H}_2\text{N--}\text{C--}\text{CH}_2\text{--}\text{CH--}\text{Et} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1967 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:102645

REFERENCE 2: 129:316688

L40 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 214783-26-3 REGISTRY

CN Pentanamide, 5-amino-4-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C6 H14 N2 O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE) 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:102645

REFERENCE 2: 129:316688

L40 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 102831-39-0 REGISTRY

CN 2-Butenamide, 4-amino-3-methyl-, monohydrochloride (9CI) (CF

INDEX NAME)

MF C5 H10 N2 O . C1 H

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

$$\begin{array}{ccc} & & \text{Me} \\ & || & & | \\ \text{H}_2\text{N}-\text{C}-\text{CH} & = \text{C}-\text{CH}_2-\text{NH}_2 \end{array}$$

● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:60922

=> d his 140-

(FILE 'REGISTRY' ENTERED AT 09:52:55 ON 12 FEB 2002)

L40 3 S L37-L39

FILE 'HCAOLD' ENTERED AT 11:34:11 ON 12 FEB 2002

L41 0 S L40

FILE 'HCAPLUS' ENTERED AT 11:34:14 ON 12 FEB 2002

L42 3 S L40

FILE 'USPATFULL, USPAT2' ENTERED AT 11:34:28 ON 12 FEB 2002

L43

1 S L40

FILE 'REGISTRY' ENTERED AT 11:34:46 ON 12 FEB 2002 => fil uspatall FILE 'USPATFULL' ENTERED AT 11:35:22 ON 12 FEB 2002 CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS) FILE 'USPAT2' ENTERED AT 11:35:22 ON 12 FEB 2002 CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS) => d 143 bib abs hitstr L43 ANSWER 1 OF 1 USPATFULL 1999:81945 USPATFULL TIEpsilon caprolactam compositions Maher, John Michael, Charleston, WV, United States TN Bryant, David Robert, South Charleston, WV, United States Holladay, Johnathan Eugene, Charleston, WV, United States Eisenschmid, Thomas Carl, Cross Lanes, WV, United States Briggs, John Robert, Charleston, WV, United States Olson, Kurt Damar, Cross Lanes, WV, United States Union Carbide Chemicals & Plastics Technology Corporation, Danbury, CT, PΑ United States (U.S. corporation) 19990720 PΤ US 5925754 ΑI US 1997-956745 19971023 (8) Continuation-in-part of Ser. No. US 1997-839576, filed on 15 Apr 1997 RLI And Ser. No. US 1997-843340, filed on 15 Apr 1997 DT FS Granted EXNAM LREP Coon, Gerald L.

Primary Examiner: Raymond, Richard L.; Assistant Examiner: Kifle, Bruck

CLMN Number of Claims: 9 Exemplary Claim: 1 ECL

DRWN No Drawings

LN.CNT 1451

AB

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

This invention relates to a composition comprising (a) epsilon caprolactam and (b) one or more of 5-[4,5-di(3-carboxypropyl)-2pyridyl]pentanoic acid or salt or amide, 4-[4,5-di(2-carboxypropyl)-2pyridyl]-2-methylbutanoic acid or salt or amide, 2-[2-(2-carboxybutyl)-5-(1-carboxypropyl)-4-pyridyl]butanoic acid or salt or amide, 5-[3,5-di(3-carboxypropyl)-2-pyridyl]pentanoic acid or salt or amide, 4-[3,5-di(2-carboxypropyl)-2-pyridyl]-2-methylbutanoic acid or salt or amide, 2-[-2-(2-carboxybutyl)-5-(1-carboxypropyl)-3-pyridyl]butanoic acid or salt or amide, 5-amino-4-methylpentanamide, 4-amino-3ethylbutanamide, 5-[4,5-di(4-hydroxybutyl)-2-pyridyl]pentanol, 4-[4,5-di(2-methoxypropyl)-2-pyridyl]-2-methylbutanol, 2-[2-(2-methoxybutyl)-5-(1-methoxypropyl)-4-pyridyl]butanol, 5-[3,5-di(4-hydroxybutyl)-2-pyridyl]pentanol, 4-[3,5-di(2-methoxypropyl)-2-pyridyl]-2-methylbutanol, 2-[2-(2-methoxybutyl)-5-(1-methoxypropyl)-3pyridyl]butanol, 5-amino-4-methyl-1-pentanol, 5-imino-2-methyl-1pentanamine, 5-amino-2-methyl-1-pentanol, 5-imino-4-methyl-1-pentanamine and 2-butyl-4,5-dipropylpyridine, wherein the weight ratio of component (a) to component (b) is at least about 99 to 1. The epsilon caprolactam compositions are useful in the preparation of nylon 6.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

214783-26-3P 214783-27-4P

(prodn. of caprolactam compns. contg. different byproducts)

RŃ 214783-26-3 USPATFULL

Pentanamide, 5-amino-4-methyl- (9CI) (CA INDEX NAME) CN

RN 214783-27-4 USPATFULL

CN Pentanamide, 3-(aminomethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} & \text{CH}_2\text{--}\text{NH}_2 \\ \parallel & \parallel \\ \text{H}_2\text{N--}\text{C--}\text{CH}_2\text{--}\text{CH--}\text{Et} \end{array}$$

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 11:35:35 ON 12 FEB 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 8 Feb 2002 VOL 136 ISS 7 FILE LAST UPDATED: 30 Jan 2002 (20020130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> d 142 bib abs hitstr retable tot

L42 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS

AN 1999:450917 HCAPLUS

DN 131:102645

TI Production of caprolactam compositions containing different byproducts for easier separation

IN Maher, John Michael; Bryant, David Robert; Holladay, Johnathan Eugene; Eisenschmid, Thomas Carl; Briggs, John Robert; Olson, Kurt Damar

PA Union Carbide Chemicals & Plastics Technology Corporation, USA

SO U.S., 15 pp. CODEN: USXXAM

DT Patent

LA English

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FAN.CNT 6
                                            APPLICATION NO.
                                                             DATE
     PATENT NO.
                      KIND
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                                            US 1997-956745
                                                             19971023
                            19990720
PI
     US 5925754
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                                                             19970415
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                       Α1
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                                                             19980414
         W: BR, CA, CN, JP, KP, KR, MX, PL, RU, SG
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
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                                                             19980414
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PRAI US 1997-839576
     US 1997-843340
                       A2
                            19970415
     US 1997-956745
                            19971023
                       Α
     WO 1998-US7486
                       W
                            19980414
     Title compns. comprise (a) .epsilon.-caprolactam and (b) one or more of
AR
     5-[4,5-di(3-carboxypropyl)-2-pyridyl]pentanoic acid or salt or amide,
     4-[4,5-di(2-carboxypropyl)-2-pyridyl]-2-methylbutanoic acid or salt or
     amide, 2-[2-(2-carboxybutyl)-5-(1-carboxypropyl)-4-pyridyl]butanoic acid
     or salt or amide, 5-[3,5-di(3-carboxypropyl)-2-pyridyl]pentanoic acid or
     salt or amide, 4-[3,5-di(2-carboxypropyl)-2-pyridyl]-2-methylbutanoic acid
     or salt or amide, 2-[2-(2-carboxybutyl)-5-(1-carboxypropyl)-3-
     pyridyl]butanoic acid or salt or amide, 5-amino-4-methylpentanamide,
     4-amino-3-ethylbutanamide, 5-[4,5-di(4-hydroxybutyl)-2-pyridyl]pentanol,
     4-[4,5-di(2-methoxypropyl)-2-pyridyl]-2-methylbutanol,
     2-[2-(2-methoxybutyl)-5-(1-methoxypropyl)-4-pyridyl]butanol,
     5-[3,5-di(4-hydroxybutyl)-2-pyridyl]pentanol, 4-[3,5-di(2-methoxypropyl)-2-
     pyridyl]-2-methylbutanol, 2-[2-(2-methoxybutyl)-5-(1-methoxypropyl)-3-
     pyridyl]butanol, 5-amino-4-methyl-1-pentanol, 5-imino-2-methyl-1-
     pentanamine, 5-amino-2-methyl-1-pentanol, 5-imino-4-methyl-1-pentanamine
     and 2-butyl-4,5-dipropylpyridine, in a:b wt. ratio at least about 99 to 1.
     The byproducts result from reductive amination and cyclization of C6
     difunctional intermediates produced by carbonylation of butadiene.
     .epsilon.-caprolactam compns. are useful in the prepn. of nylon 6.
ΙT
     214783-26-3P 214783-27-4P
     RL: BYP (Byproduct); PREP (Preparation)
        (prodn. of caprolactam compns. contg. different byproducts)
RN
     214783-26-3 HCAPLUS
     Pentanamide, 5-amino-4-methyl- (9CI) (CA INDEX NAME)
CN
```

RN214783-27-4 HCAPLUS Pentanamide, 3-(aminomethyl)- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c} \text{O} & \text{CH}_2\text{--}\text{NH}_2 \\ \parallel & \parallel \\ \text{H}_2\text{N--}\text{C--}\text{CH}_2\text{--}\text{CH--}\text{Et} \end{array}$$

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Referenced Author	Year	(RWK)	File ····
Anon Anon Anon Anon	1971 1974 1984	GB 1254222 GB 1357735 RU 1087510 EP 0183545	HCAPLUS HCAPLUS HCAPLUS

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Anon	1987	1	EP 0271145	HCAPLUS
	1988	i	EP 0273489	HCAPLUS
	1989	i	IEP 0343819	HCAPLUS
	1990	i	EP 0351616	HCAPLUS
	1990	i	IEP 0405433	HCAPLUS
	11991	İ	EP 0420510	HCAPLUS
	1991	ĺ	EP 0448848	HCAPLUS
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Anon	1993	i ·	EP 0556681	HCAPLUS
	1993	İ	EP 0562450	HCAPLUS
	1993	Ì	EP 0577205	HCAPLUS
	1993 .	i	JP 06306012	HCAPLUS
	1994		IEP 0602442	HCAPLUS
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	11995	i	WO 9518089	HCAPLUS
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Anon	1996	İ	EP 0738701	HCAPLUS
	1997	ĺ	EP 0761634	HCAPLUS
	1994	j	US 5292944	HCAPLUS
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	1990		US 4910328	HCAPLUS
Bertleff	1991		US 5003102	HCAPLUS
Bertozzi, S	1995 487	41	Journal of Organomet	HCAPLUS
Billig	1988		US 4769498	HCAPLUS
Botteghi, C	1980 184	C17	Journal of Organomet	HCAPLUS
Bunel	1994		US 5288903	HCAPLUS
Burke	1986	1	US 4622423	HCAPLUS
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Carlock	1980	1	US 4185083	HCAPLUS
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	1995	1	US 5434312	HCAPLUS
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9	1972	1	US 36525 4 9	HCAPLUS
	1987	1	US 4658068	HCAPLUS
	1980	1	US 4200591	HCAPLUS
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Van Leeuwen, P
                        |1985 |31
                                            |US 4647707
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L42
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ΤI
     Epsilon caprolactam compositions and byproducts
IN
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     Eisenschmid, Thomas Carl; Briggs, John Robert; Olson, Kurt Damar
PΑ
     Union Carbide Chemicals & Plastics Technology Corp., USA
SO
     PCT Int. Appl., 51 pp.
     CODEN: PIXXD2
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                                             APPLICATION NO.
     PATENT NO.
                       KIND
                             DATE
                                                               DATE
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     WO 9846564
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                             19971023
                        Α
     WO 1998-US7486
                        W
                             19980414
     This invention relates to a compn. comprising (a) epsilon caprolactam and
AB
     (b) one or more of 5-[4,5-di(3-carboxypropyl)-2-pyridyl]pentanoic acid or
     salt or amide, 4-[4,5-di(2-carboxypropyl)-2-pyridyl]-2-methylbutanoic acid
     or salt or amide, 2-[2-(2-carboxybutyl)-5-(1-carboxypropyl)-4-
     pyridyl]butanoic acid or salt or amide, 5-[3,5-di(3-carboxypropyl)-2-
     pyridyl]pentanoic acid or salt or amide, 4-[3,5-di(2-carboxypropyl)-2-
```

pyridyl]-2-methylbutanoic acid or salt or amide, 2-[2-(2-carboxybutyl)-5-

(1-carboxypropyl)-3-pyridyl]butanoic acid or salt or amide, 5-amino-4-methylpentanamide, 4-amino-3-ethylbutanamide, 5-[4,5-di(4-hydroxybutyl)-2-pyridyl]pentanol, 4-[4,5-di(2-methoxypropyl)-2pyridyl]-2-methylbutanol, 2-[2-(2-methoxybutyl)-5-(1-methoxypropyl)-4pyridyl]butanol, 5-[3,5-di(4-hydroxybutyl)-2-pyridyl]pentanol, 4-[3,5-di(2-methoxypropyl)-2-pyridyl]-2-methylbutanol, 2[2-(2-methoxybutyl)-5-(1-methoxypropyl)-3-pyridyl]butanol, 5-amino-4-methyl-1-pentanol, 5-imino-2-methyl-1-pentanamine, 5-amino-2-methyl-1-pentanol, 5-imino-4-methyl-1-pentanamine and 2-butyl-4,5-dipropylpyridine, wherein the wt. ratio of component a) to component b) is at least about 99 to 1. The epsilon caprolactam compns. are useful in the prepn. of nylon 6.

214783-26-3P 214783-27-4P ΙT

> RL: BYP (Byproduct); PREP (Preparation) (epsilon caprolactam compns. and byproducts)

RN 214783-26-3 HCAPLUS

CN Pentanamide, 5-amino-4-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{ccc} & & & \text{Me} \\ || & & | \\ \text{H}_2\text{N--C-CH}_2\text{--CH}_2\text{--CH--CH}_2\text{--NH}_2 \end{array}$$

RN 214783-27-4 HCAPLUS

CN Pentanamide, 3-(aminomethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{O} & \mathsf{CH}_2 - \mathsf{NH}_2 \\ \parallel & \parallel \\ \mathsf{H}_2 \mathsf{N} - \mathsf{C} - \mathsf{CH}_2 - \mathsf{CH} - \mathsf{Et} \end{array}$$

L42 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS

ΑN 1986:460922 HCAPLUS

DN 105:60922

TΤ .beta.-Methyleneglutamic acid and .beta.-methyleneglutamine

ΑU Paik, Yi Hyon; Dowd, Paul

CS Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA

SO J. Org. Chem. (1986), 51(15), 2910-13

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 105:60922

GI

$$H_2N$$
 CO_2H EtO_2C CO_2Et H_2N H_2C Me COR I R^2 II COR III

AB Title compds. DL-I (R = OH and NH2, resp.) were prepd. from aminomalonates and allenes. Thus, AcNHCH(CO2Et)2 was treated with HgC:C:CHCO2Et in the presence of EtONa to give adduct II (R1 = Ac, R2 = CO2Et), which was hydrolyzed by 20% HCl at 50.degree. to give DL-I.cntdot.HCl (R = OH) and unsatd. acid III.cntdot.HCl (R = OH). Also, BocNHCH(CO2Et)2 (Boc = Me3CO2C) was treated with H2C:C:CHCN in the presence of EtONa to give II (R1 = Boc, R2 = CN), which was hydrolyzed by 20% HCl at 50 degree to give DL-I.cntdot.HCl (R = NH2) and unsatd. amide III (R = NH2).

IT

L29

4354 S L11 NOT (L24 OR L27) FUL

102831-39-0P

```
RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     102831-39-0 HCAPLUS
CN
     2-Butenamide, 4-amino-3-methyl-, monohydrochloride (9CI) (CA INDEX NAME)
           Me
H2N-C-CH C-CH2-NH2
        HC1
=> d his
     (FILE 'HOME' ENTERED AT 09:48:46 ON 12 FEB 2002)
                SET COST OFF
     FILE 'HCAPLUS' ENTERED AT 09:49:03 ON 12 FEB 2002
                E WELLS I/AU
L1
             52 S E3, E4, E14
                E MAGNESIUM/CS, PA
L2
              0 S (MAGNES?(L)DIAG?)/PA,CS
L3
              9 S L1 AND (MAGNESIUM OR MG###)
     FILE 'REGISTRY' ENTERED AT 09:51:04 ON 12 FEB 2002
              1 S 7439-95-4
L4
     FILE 'HCAPLUS' ENTERED AT 09:51:31 ON 12 FEB 2002
L5
              2 S L4 AND L1
              9 S L3, L5
L6
     FILE 'REGISTRY' ENTERED AT 09:51:56 ON 12 FEB 2002
              1 S 22537-22-0
L7
                E MAGNESIUM, ION/CN
rs
              1 S E4
     FILE 'HCAPLUS' ENTERED AT 09:52:30 ON 12 FEB 2002
L9
              1 S L7, L8 AND L1
L10
              9 S L6, L9
     FILE 'REGISTRY' ENTERED AT 09:52:55 ON 12 FEB 2002
L11
               STR
L12
             30 S L11
L13
               STR L11
L14
              4 S L13
L15
                SCR 2043 OR 2127
L16
              5 S L13 NOT L15
L17
                SCR 2039 OR 2127 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 205
L18
              3 S L13 NOT L17
L19
                STR L13
L20
              3 S L19 NOT L17
L21
                STR L19
L22
             0 S L21 NOT L17 CSS SAM
L23
             17 S L11 NOT L17 SAM
           SCR 2016 OR 2026 OR 1997 OR 1841
L24
L25
             12 S L11 NOT (L17 OR L24)
L26
              0 S L21 NOT (L17 OR L24) CSS SAM
L27
                SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 OR 204
             14 S L11 NOT (L24 OR L27)
L28
```

```
SAV KUMAR635/A L29
L30
              0 S L21 CSS SAM SUB=L29
L31
             23 S L21 SAM SUB=L29
L32
              0 S L21 CSS FUL SUB=L29
L33
                STR L19
L34
              4 S L33 CSS SAM SUB=L29
             84 S L33 CSS FUL SUB=L29
L35
                SAV L35 KUMAR635A/A
L36
             12 S L35 AND (C6H14N2O OR C5H10N2O)
              1 S L36 AND PENTANAMIDE AND AMINOMETHYL
L37
              1 S L36 AND PENTANAMIDE AND 5 AMINO 4 METHYL
L38
              1 S L36 AND BUTENAMIDE
L39
              3 S L37-L39
L40
```

FILE 'HCAOLD' ENTERED AT 11:34:11 ON 12 FEB 2002 L41 0 S L40

FILE 'HCAPLUS' ENTERED AT 11:34:14 ON 12 FEB 2002 L42 3 S L40

FILE 'USPATFULL, USPAT2' ENTERED AT 11:34:28 ON 12 FEB 2002 L43

=> fil reg FILE 'REGISTRY' ENTERED AT 12:30:03 ON 12 FEB 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9 DICTIONARY FILE UPDATES: 10 FEB 2002 HIGHEST RN 391197-12-9

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> d sta que 18

L1 STR

CH— CH2— CH @15 16 @17 CH—CH2—CH2—CH @18 19 20 @21 NH—Ak 022 23 Ak— N— Ak 24 @25 26

VAR G1=7-2 10-4/11-2 12-4/13-2 14-4/15-2 17-4/18-2 21-4

VAR G2=NH2/22/25

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 23

CONNECT IS E1 RC AT 24

CONNECT IS E1 RC AT 2

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

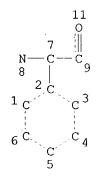
L2 SCR 2016 OR 2026 OR 1997 OR 1841

L3 SCR 2039 OR 2050 OR 2049 OR 2048 OR 2053 OR 2052 OR 2051 O

R 2043 OR 2054

L4 4354 SEA FILE=REGISTRY SSS FUL L1 NOT (L2 OR L3)

L5 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L7 17 SEA FILE=REGISTRY SUB=L4 SSS FUL L5

L8 3 SEA FILE=REGISTRY ABB=ON PLU=ON L7 AND NA/ELS:

 \Rightarrow d his 18-

(FILE 'REGISTRY' ENTERED AT 12:24:47 ON 12 FEB 2002)

SAV L7 KUMAR635B/A

L8 3 S L7 AND NA/ELS

FILE 'HCAOLD' ENTERED AT 12:29:22 ON 12 FEB 2002

L9 ' 0 S L8

FILE 'HCAPLUS' ENTERED AT 12:29:26 ON 12 FEB 2002 L10 2 S L8

FILE 'USPATFULL, USPAT2' ENTERED AT 12:29:43 ON 12 FEB 2002 L11 0 S L8

FILE 'REGISTRY' ENTERED AT 12:30:03 ON 12 FEB 2002

=> d ide can tot 18

L8 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 61544-14-7 REGISTRY

CN Benzeneacetic acid, .alpha.-[[4-(dimethylamino)-2-methyl-4-oxo-2-butenyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzeneacetic acid, .alpha.-[[4-(dimethylamino)-2-methyl-4-oxo-2-butenyl]amino]-, monosodium salt, (.+-.)-

MF C15 H20 N2 O3 . Na

LC STN Files: CA, CAPLUS

Na

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:55412

L8 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 50971-89-6 REGISTRY

CN Benzeneacetic acid, .alpha.-[[4-(dimethylamino)-4-oxo-2-butenyl]amino]-4-hydroxy-, monosodium salt (9CI) (CA INDEX NAME)

MF C14 H18 N2 O4 . Na

LC STN Files: CA, CAPLUS

Na

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFÉRENCE 1: 80:14945

L8 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2002 ACS

RN 50971-87-4 REGISTRY

CN Benzeneacetic acid, .alpha.=[[4-(dimethylamino)-4-oxo-2-butenyl]amino]-,
 monosodium salt (9CI) (CA INDEX NAME)

IF C14 H18 N2 O3 . Na

LC STN Files: CA, CAPLUS

Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 80:14945

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FILE COVERS 1907 - 8 Feb 2002 VOL 136 ISS 7 FILE LAST UPDATED: 30 Jan 2002 (20020130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> d bib abs hitstr retable tot 110

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS

AN 1977:55412 HCAPLUS

DN 86:55412

TI DL-6-Aminoacylamidopenicillanic acids

PA Osaka University, Japan

SO Ger. Offen., 24 pp. Division of Ger. Offen. 2,020,133.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 2

1. 2-	IIV. CIVI Z				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
				-	
ΡI	DE 2065879	A1	19760826	DE 1970-2065879	19700424
	NL 7005611	A	19701103	NL 1970-5611	19700417
	DK 132026	В	19751013	DK 1970-2079	19700423
	ES 379011	A1	19720801	ES 1970-379011	19700424
	FR 2040451	A5	19710122	FR 1970-15647	19700429
	NL 7402745	A	19740527	NL 1974-2745	19740228
	NL 164020	В	19800616		
	NL 164020	C	19801117		
PF	AI JP 1969-33867		19690430		
GI					

AB 6-(Aminoacylamido)penicillanic acid [I; R = PhCH(NH2),
.alpha.-amino-2-thenyl, (MeS)CH2CH2CH(NH2), 1-aminocyclohexyl] are prepd.
by reaction of 6-aminopenicillanic acid (II) with amino acid derivs.,
protected on the N with a .beta.-keto acid deriv. Thus,
aminobenzylpenicillin [I; R = PhCH(NH2)] is obtained in 60% yield by
condensation of II with the mixed anhydride from pivalic acid and
[[1-methyl-2-(morpholinocarbonyl)vinyl]amino]phenylacetic acid.

IT 61544-14-7

RL: RCT (Reactant)

(acylation by, of 6-aminopenicillanic acid)

RN 61544-14-7 HCAPLUS

CN Benzeneacetic acid, .alpha.-[[4-(dimethylamino)-2-methyl-4-oxo-2-butenyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)

Na

L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS AN 1974:14945 HCAPLUS

DN 80:14945

TI Cephalosporins

IN Ishimaru, Toshiyasu; Kodama, Yutaka

PA Toyoma Chemical Co., Ltd.

SO Fr. Demande, 12 pp. CODEN: FRXXBL

DT Patent

LA French

FAN.	CNT 1			•	
	PATENT NO.	KIND.	DATE	APPLICATION NO.	DATE
PI	FR 2166316	A1	19730817	FR 1972-514	19720107
	FR 2166316	В1	19771028		
GĮ	For diagram(s),	see pr	inted CA Issue.		

Cephalosporins I (R = 2-thienylacetyl, PhCH(NH2)CO, p-HOC6H4CH(NH2)CO; R1 = OAc, OMe, H) were prepd. by acylating I (R = H) in the presence of methoxysilyl chloride R2(MeO)2SiCl (R2 = Me, MeO), or R3(MeO)SiCl2 (R3 = Me, Ph, MeO). Thus I (R = H, R1 = OAc) was treated with Me-(MeO)2SiCl,

followed by 2-thienylacetyl chloride and HCl to give 86% I (R = 2-thienylacetyl, R1 = OAc) as its Na salt.

IT 50971-87-4 50971-89-6 RL: RCT (Reactant)

(acylation of cephalosporins by)

RN 50971-87-4 HCAPLUS

CN Benzeneacetic acid, .alpha.-[[4-(dimethylamino)-4-oxo-2-butenyl]amino]-, monosodium salt (9CI) (CA INDEX NAME)

Na

CN Benzeneacetic acid, .alpha.-[[4-(dimethylamino)-4-oxo-2-butenyl]amino]-4-hydroxy-, monosodium salt (9CI) (CA INDEX NAME)

● Na